10552362a

Enter NEWS followed by the item number or name to see news on that
specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:20:17 ON 02 APR 2007

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'REGISTRY' ENTERED AT 14:20:27 ON 02 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2007   HIGHEST RN 928822-97-3
DICTIONARY FILE UPDATES: 1 APR 2007   HIGHEST RN 928822-97-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

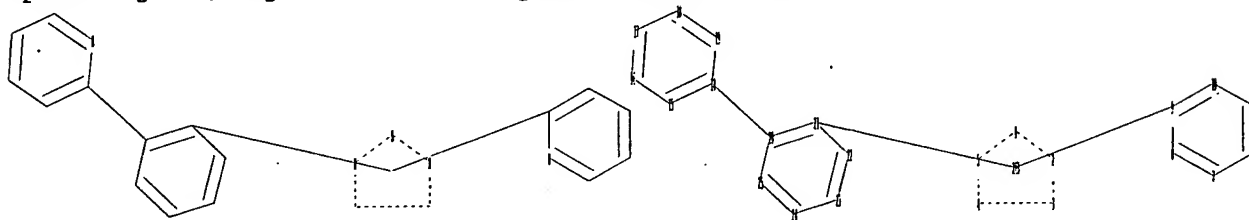TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res1.str

ring nodes :
1   2   3   4   5   7   8   9   10   11   12   14   15   16   17   18   19   20   21   22   23   24   25

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chain bonds :
14-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-21 20-25 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
14-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-21
 20-25 21-22 22-23 23-24 24-25
isolated ring systems :
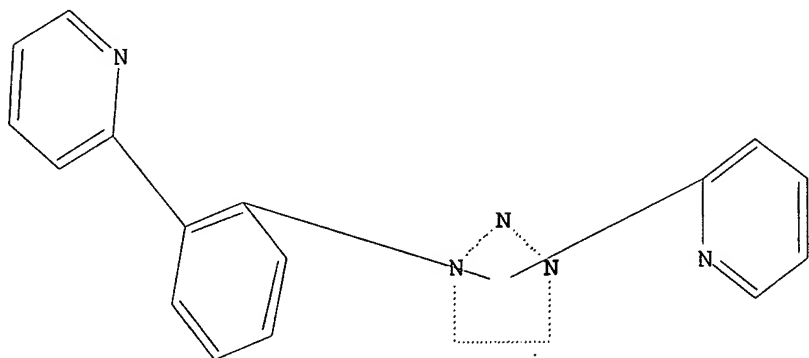containing 1 : 7 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 14:20:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1535 TO ITERATE

100.0% PROCESSED   1535 ITERATIONS   0 ANSWERS
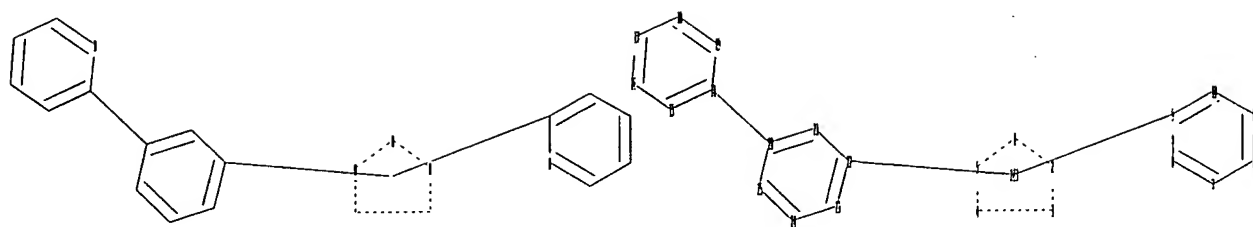SEARCH TIME: 00.00.01

L2   0 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res2.str

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```
ring nodes :
1   2   3   4   5   7   8   9   10  11  12  14  15  16  17  18  19  20  21  22  23  24  25 .
chain bonds :
14-20
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12  8-9   9-10  10-11  11-12  14-19  14-15  15-16
16-17  17-18  18-19  20-21  20-25  21-22  22-23  23-24  24-25
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
14-20
normalized bonds :
7-8   7-12  8-9   9-10  10-11  11-12  14-19  14-15  15-16  16-17  17-18  18-19  20-21
 20-25  21-22  22-23  23-24  24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :


Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom
21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom
```
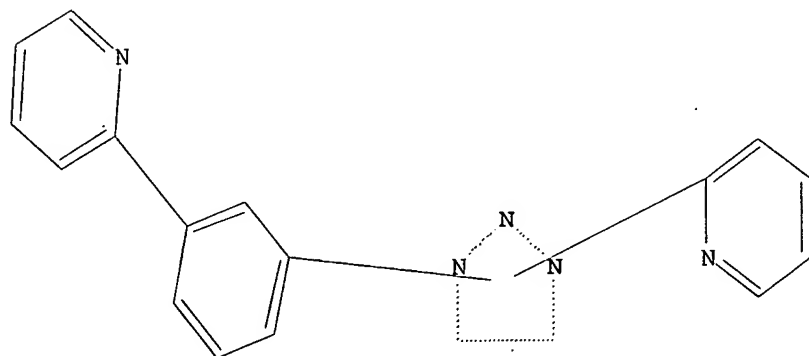
L3   STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3   STR

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Structure attributes must be viewed using STN Express query preparation.


```
=> s l3 full
FULL SEARCH INITIATED 14:21:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      1185 TO ITERATE

100.0% PROCESSED     1185 ITERATIONS                        2 ANSWERS
SEARCH TIME: 00.00.01

L4              2 SEA SSS FUL L3

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res3.str
```
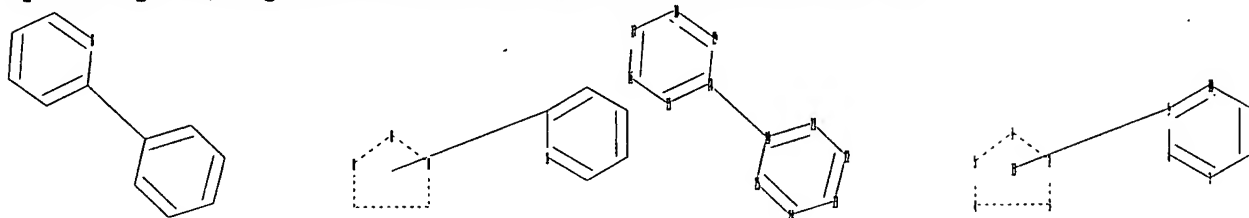


```
ring nodes :
1  2  3  4  5  7  8  9  10  11  12  14  15  16  17  18  19  20  21  22  23  24  25
chain bonds :
14-20
ring bonds :
1-2  1-5  2-3  3-4  4-5  7-8  7-12  8-9  9-10  10-11  11-12  14-19  14-15  15-16
16-17  17-18  18-19  20-21  20-25  21-22  22-23  23-24  24-25
exact/norm bonds :
1-2  1-5  2-3  3-4  4-5
exact bonds :
14-20
normalized bonds :
7-8  7-12  8-9  9-10  10-11  11-12  14-19  14-15  15-16  16-17  17-18  18-19  20-21
 20-25  21-22  22-23  23-24  24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  7:Atom  8:Atom  9:Atom  10:Atom  11:Atom
12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom
21:Atom  22:Atom  23:Atom  24:Atom  25:Atom



L5       STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5                STR
```
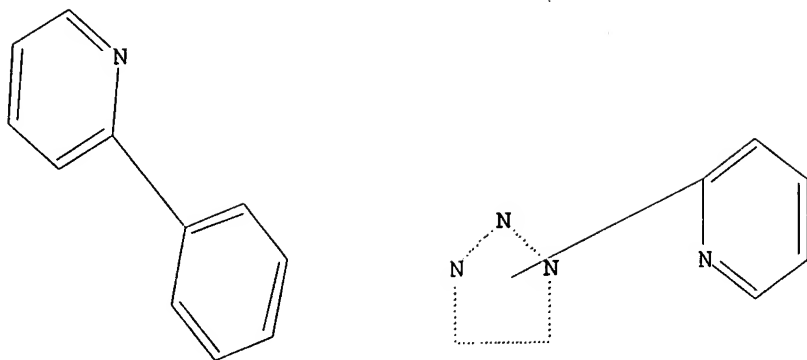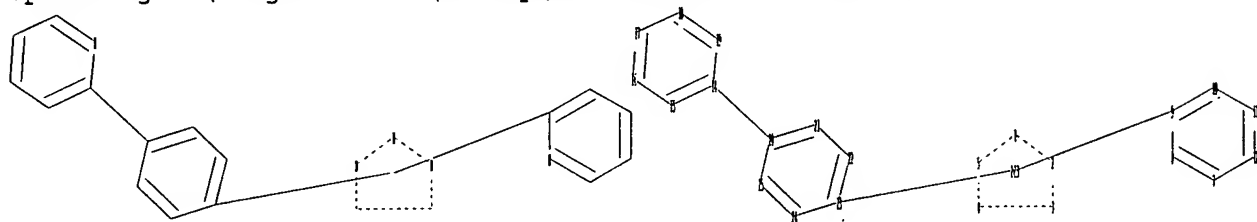

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Structure attributes must be viewed using STN Express query preparation.

```
=>
Uploading C:\Program Files\Stnexp\Queries\10552362res4.str
```



```
ring nodes :
1   2   3   4   5   7   8   9   10  11  12  14  15  16  17  18  19  20  21  22  23  24  25
chain bonds :
14-20
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12  8-9   9-10  10-11  11-12  14-19  14-15  15-16
16-17  17-18  18-19  20-21  20-25  21-22  22-23  23-24  24-25
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
14-20
normalized bonds :
7-8   7-12  8-9   9-10   10-11   11-12  14-19  14-15  15-16  16-17  17-18  18-19  20-21
 20-25  21-22  22-23  23-24  24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :


Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom  18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom
```

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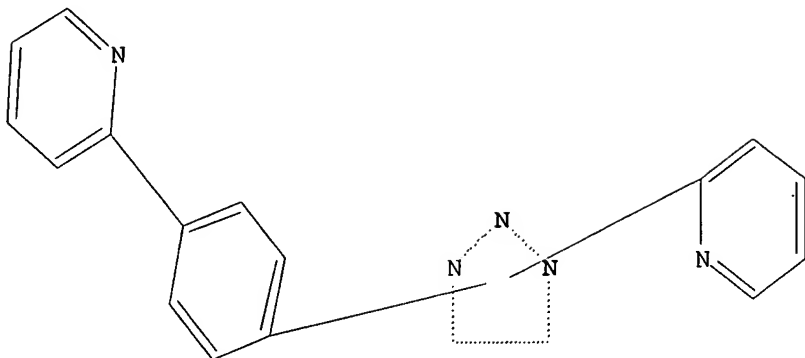
10552362a

L6   STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l6 full
FULL SEARCH INITIATED 14:23:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1185 TO ITERATE

100.0% PROCESSED   1185 ITERATIONS   8 ANSWERS
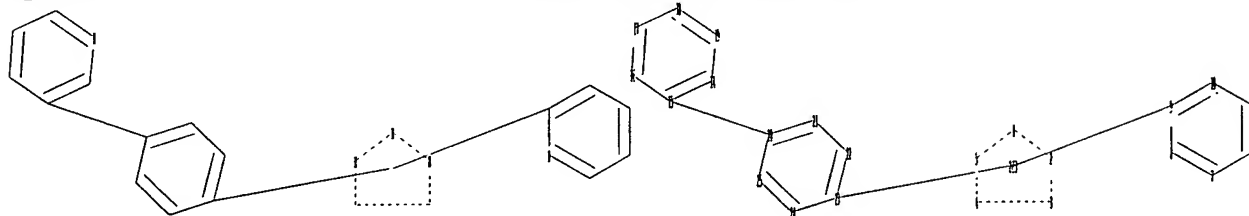SEARCH TIME: 00.00.01

L7   8 SEA SSS FUL L6

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res5.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
15-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
15-20
normalized bonds :

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7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
 20-21 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :
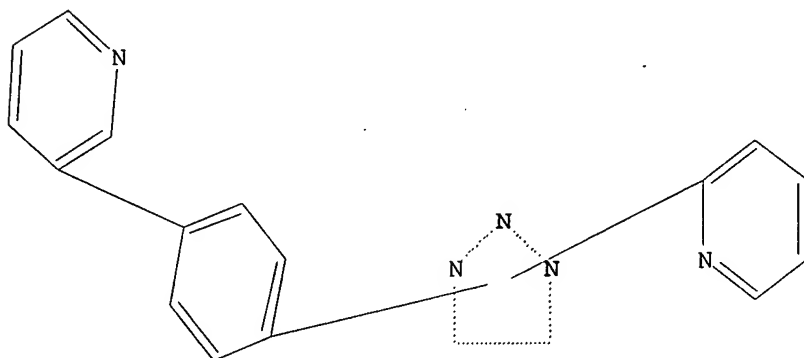

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L8   STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l8 full
FULL SEARCH INITIATED 14:24:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
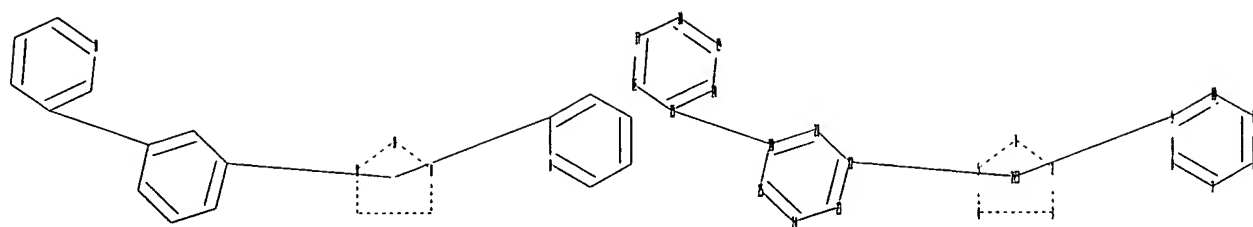SEARCH TIME: 00.00.01

L9   0 SEA SSS FUL L8

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res6.str

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ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
15-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
15-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
 20-21 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :
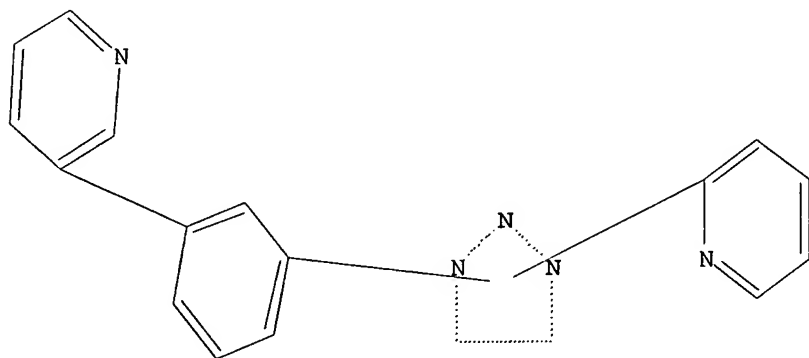

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L10   STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10   STR

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10552362a

Structure attributes must be viewed using STN Express query preparation.

=> s l10 full
FULL SEARCH INITIATED 14:25:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   2 ANSWERS
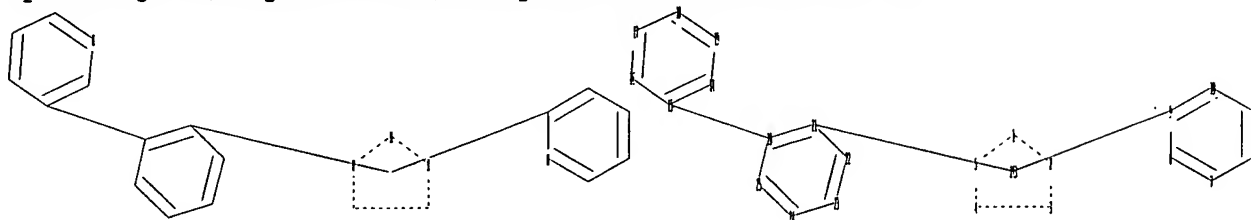SEARCH TIME: 00.00.01

L11   2 SEA SSS FUL L10

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res7.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
15-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
15-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
 20-21 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
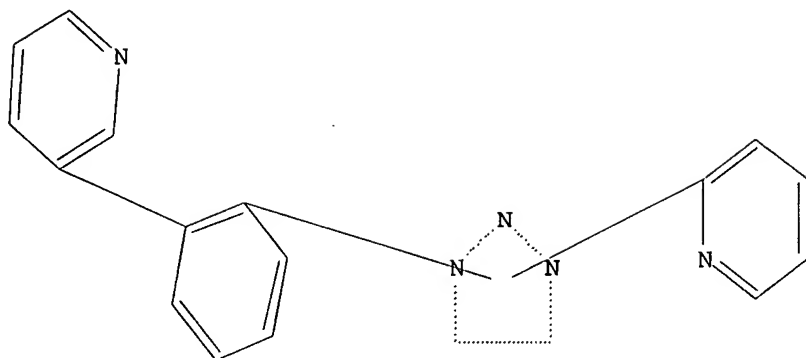

L12   STRUCTURE UPLOADED

=> d
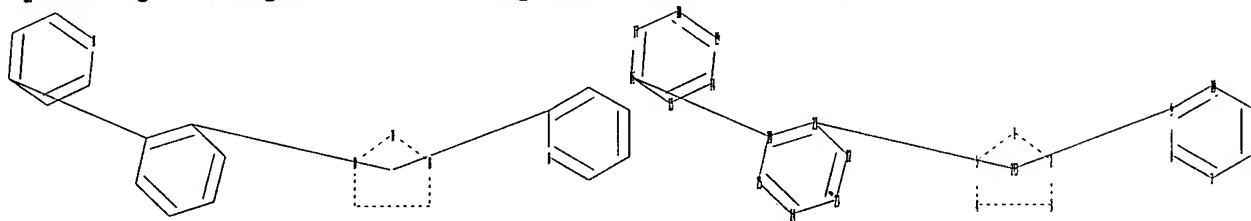L12 HAS NO ANSWERS
L12   STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l12 full
FULL SEARCH INITIATED 14:25:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L13   0 SEA SSS FUL L12

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res8.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
16-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
16-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
 20-21 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :

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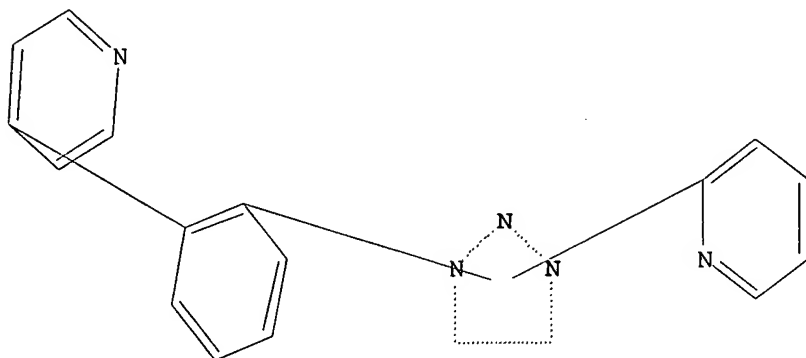Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom   20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L14   STRUCTURE UPLOADED

=> d
L14 HAS NO ANSWERS
L14   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l14 full
FULL SEARCH INITIATED 14:26:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   435 TO ITERATE

100.0% PROCESSED   435 ITERATIONS   0 ANSWERS
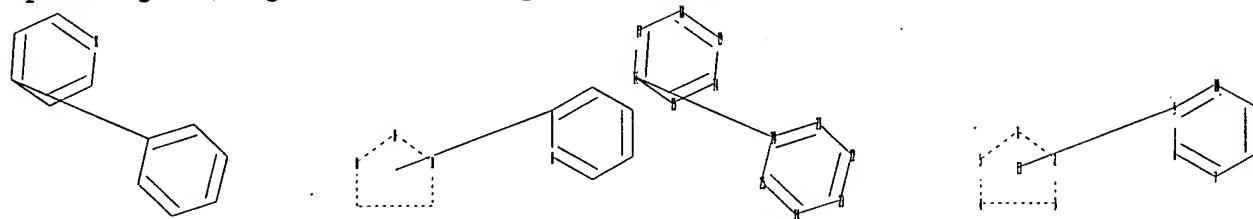SEARCH TIME: 00.00.01

L15   0 SEA SSS FUL L14

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res9.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :

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16-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
16-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
 20-21 21-22 22-23 23-24 24-25
isolated ring systems :
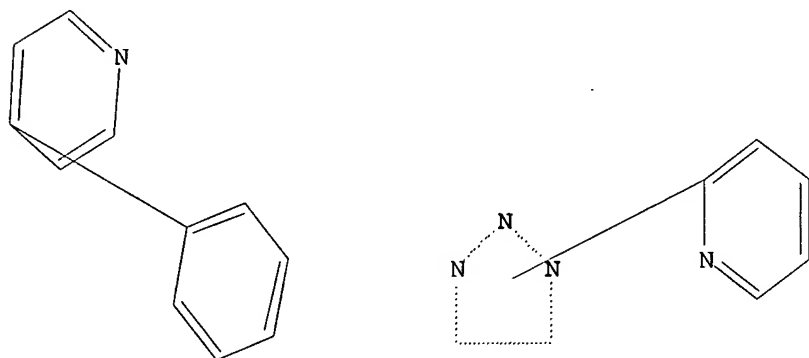containing 1 : 7 : 14 : 20 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom

L16   STRUCTURE UPLOADED

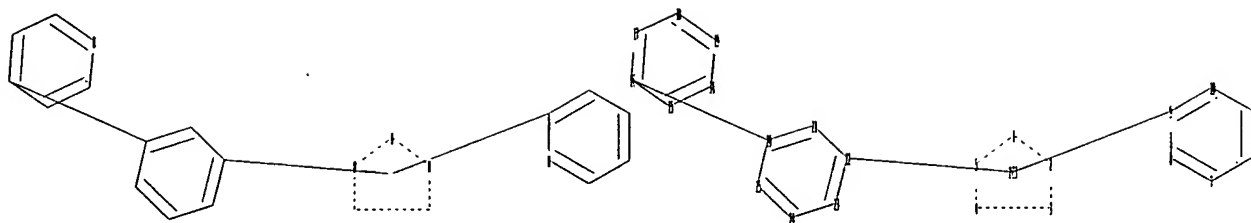=> d
L16 HAS NO ANSWERS
L16   STR

Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res10.str

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ring nodes :
1 2   3   4   5   7   8   9   10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
16-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
16-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
 20-21 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :
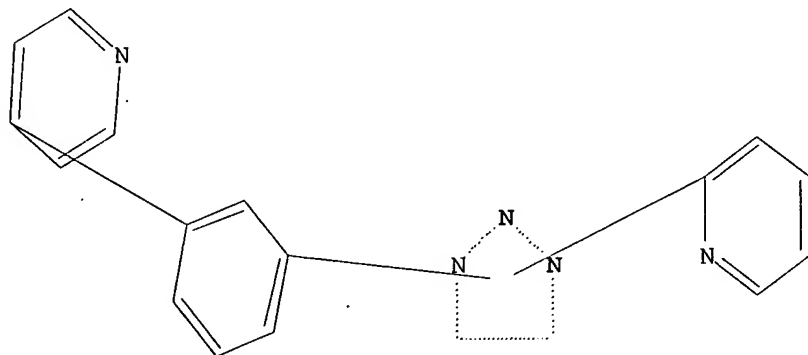

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L17   STRUCTURE UPLOADED

=> d
L17 HAS NO ANSWERS
L17   STR

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10552362a

Structure attributes must be viewed using STN Express query preparation.

=> s l17 full
FULL SEARCH INITIATED 14:28:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   435 TO ITERATE

100.0% PROCESSED   435 ITERATIONS   0 ANSWERS
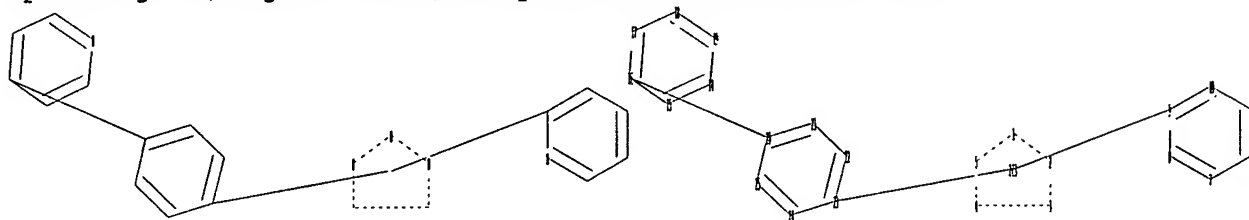SEARCH TIME: 00.00.01

L18   0 SEA SSS FUL L17

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res11.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
16-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
16-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
 20-21 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

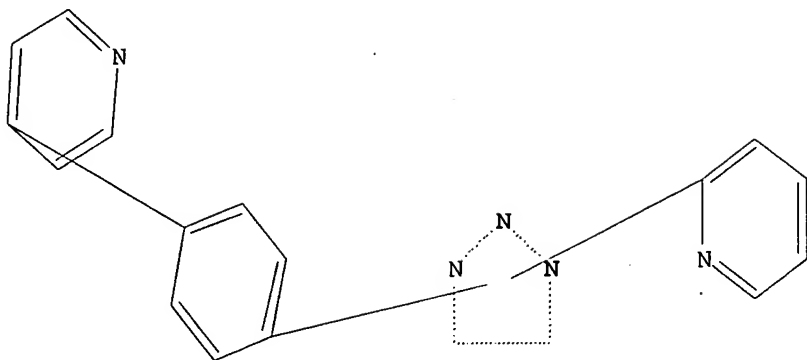L19   STRUCTURE UPLOADED

=> d
L19 HAS NO ANSWERS
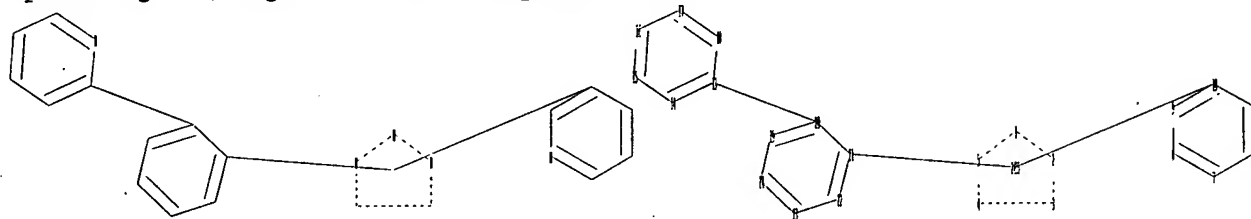L19   STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l19 full
FULL SEARCH INITIATED 14:29:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   435 TO ITERATE

100.0% PROCESSED   435 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L20   0 SEA SSS FUL L19

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res12.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
13-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
13-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

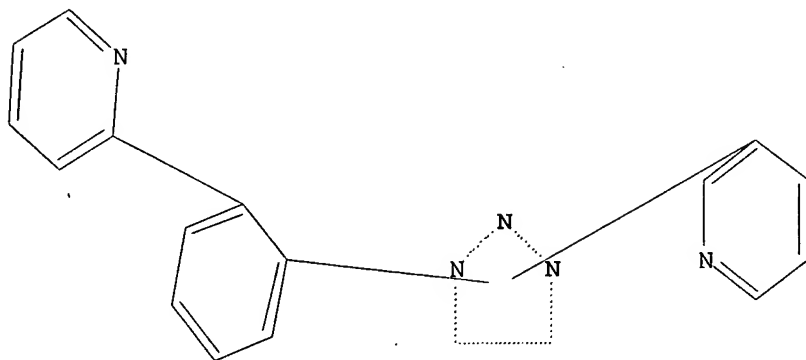Karen Cheng

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L21   STRUCTURE UPLOADED

=> d
L21 HAS NO ANSWERS
L21   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l21 full
FULL SEARCH INITIATED 14:31:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1185 TO ITERATE

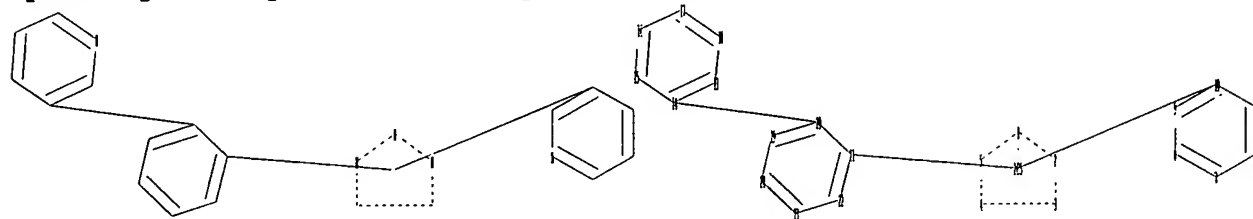100.0% PROCESSED   1185 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L22   0 SEA SSS FUL L21

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res13.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :

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14-20
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15
15-16   16-17   17-18   19-24   19-20   20-21   21-22   22-23   23-24
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
14-20
normalized bonds :
7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15   15-16   16-17   17-18   19-24
 19-20   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

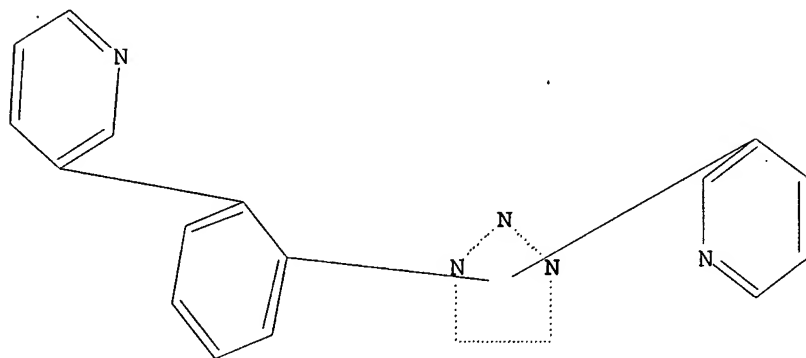Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom

L23   STRUCTURE UPLOADED

=> d
L23 HAS NO ANSWERS
L23   STR

Structure attributes must be viewed using STN Express query preparation.

=> s 123 full
FULL SEARCH INITIATED 14:31:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01
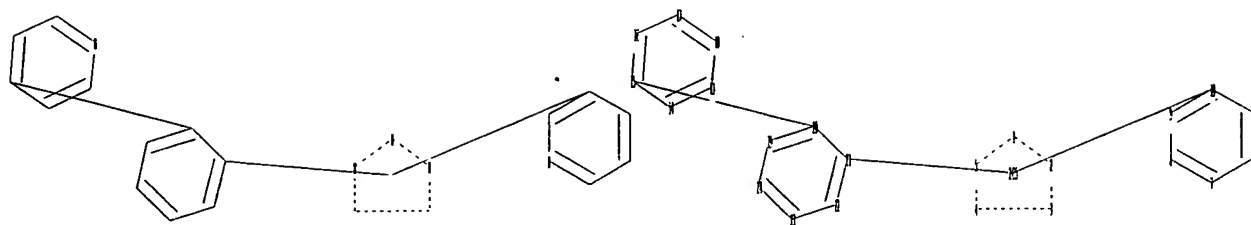
L24   0 SEA SSS FUL L23

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res14.str

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ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
15-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
15-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :
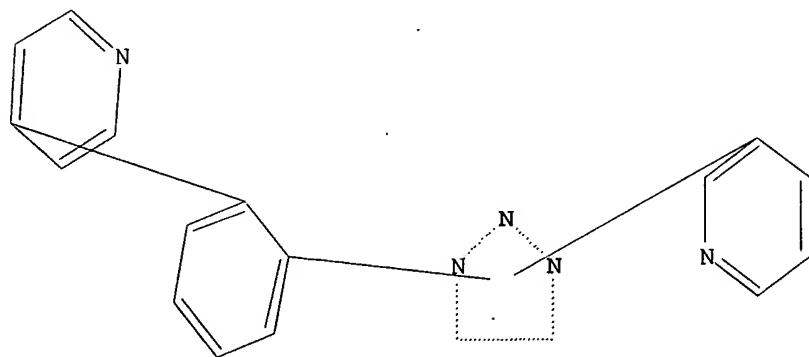

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L25   STRUCTURE UPLOADED

=> d
L25 HAS NO ANSWERS
L25   STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l25 full
FULL SEARCH INITIATED 14:32:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   435 TO ITERATE

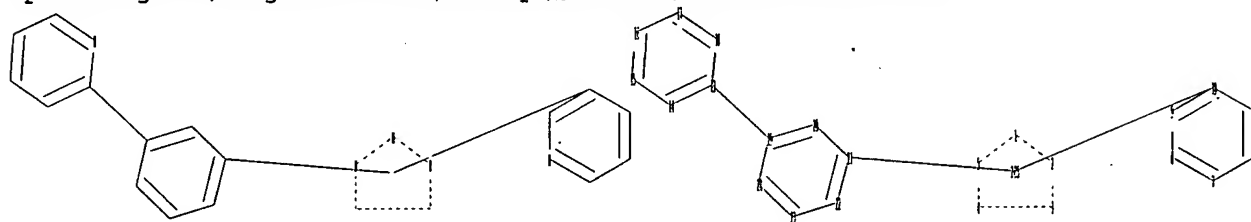100.0% PROCESSED   435 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L26   0 SEA SSS FUL L25

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res15.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
13-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
13-19
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
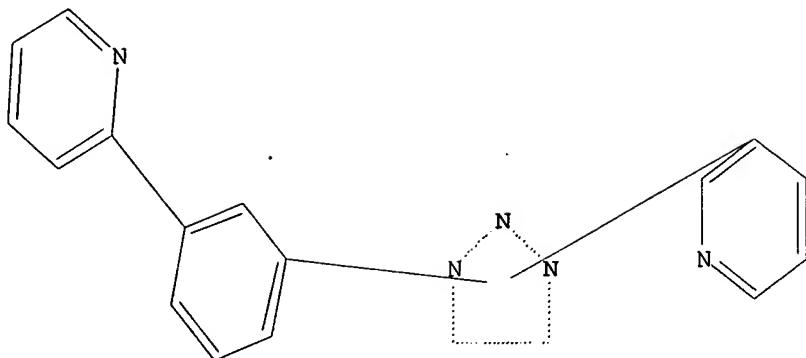

L27   STRUCTURE UPLOADED

=> d
L27 HAS NO ANSWERS
L27   STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l27 full
FULL SEARCH INITIATED 14:33:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1185 TO ITERATE

100.0% PROCESSED   1185 ITERATIONS   0 ANSWERS
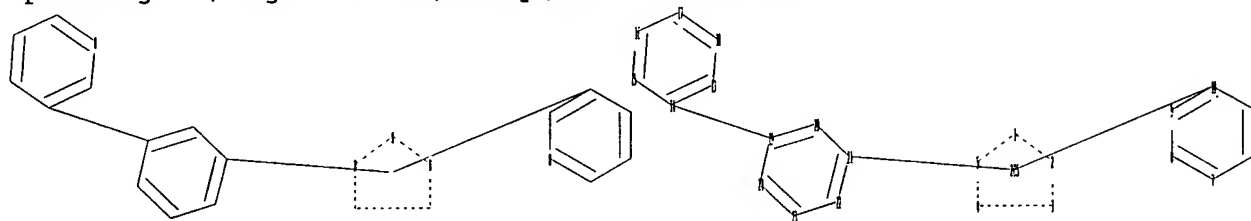SEARCH TIME: 00.00.01

L28   0 SEA SSS FUL L27

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res16.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
14-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
14-19
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

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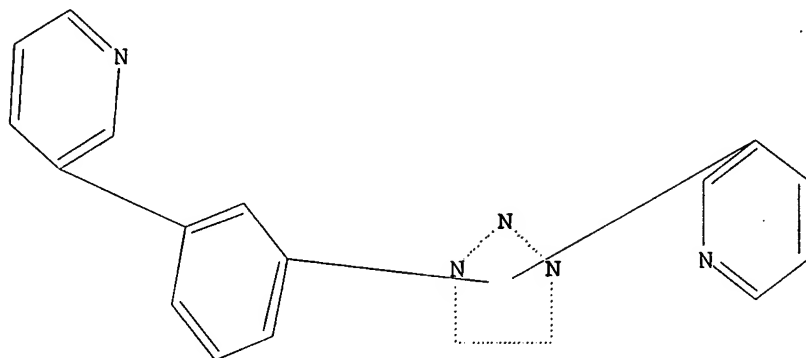Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom

L29   STRUCTURE UPLOADED

=> d
L29 HAS NO ANSWERS
L29   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l29 full
FULL SEARCH INITIATED 14:33:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

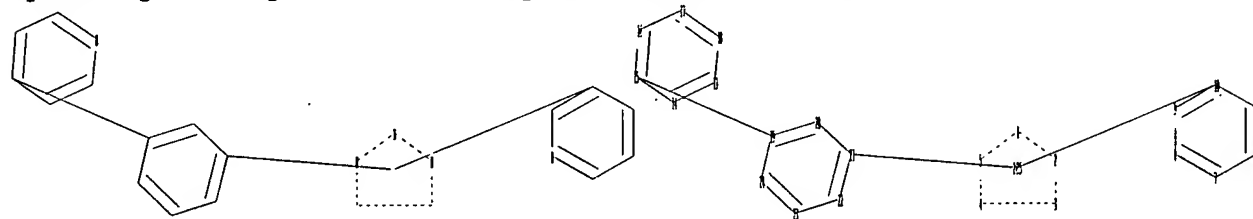100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L30   0 SEA SSS FUL L29

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res17.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :

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15-19
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15
15-16   16-17   17-18   19-24   19-20   20-21   21-22   22-23   23-24
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
15-19
normalized bonds :
7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15   15-16   16-17   17-18   19-24
 19-20   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom

L31   STRUCTURE UPLOADED

=> s l31 full
FULL SEARCH INITIATED 14:34:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   435 TO ITERATE

100.0% PROCESSED   435 ITERATIONS   0 ANSWERS
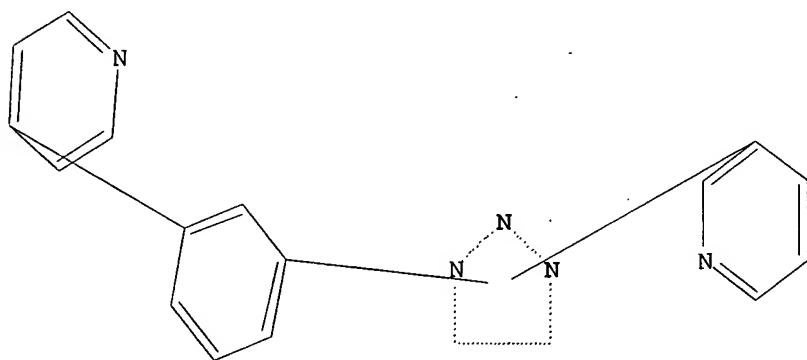SEARCH TIME: 00.00.01

L32   0 SEA SSS FUL L31

=> d
L32 HAS NO ANSWERS
L31   STR

Structure attributes must be viewed using STN Express query preparation.
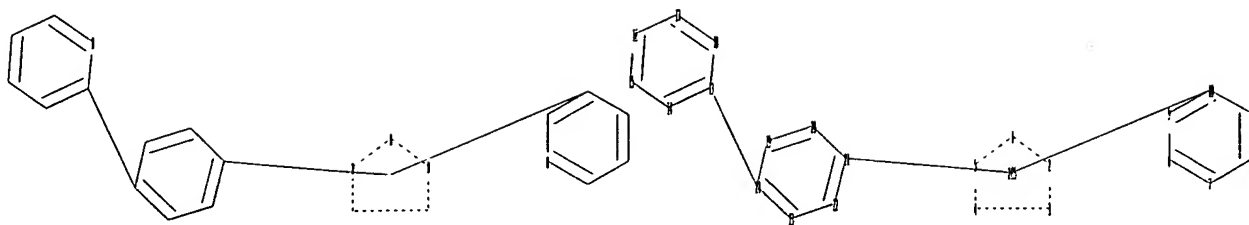L32   0 SEA FILE=REGISTRY SSS FUL L31

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res18.str

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ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
13-24
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15
15-16   16-17   17-18   19-24   19-20   20-21   21-22   22-23   23-24
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
13-24
normalized bonds :
7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15   15-16   16-17   17-18   19-24
 19-20   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

Match level :
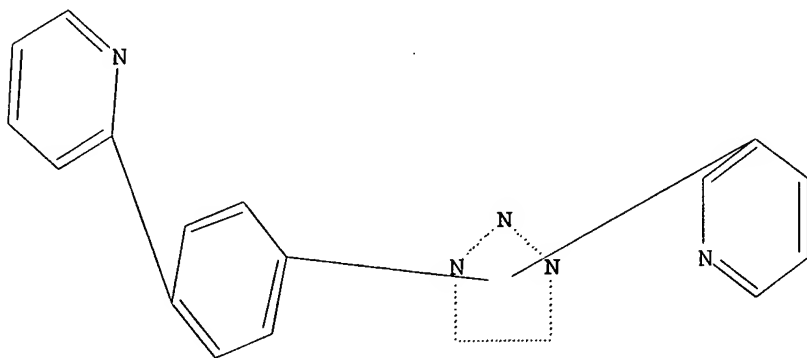1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom

L33   STRUCTURE UPLOADED

=> d
L33 HAS NO ANSWERS
L33   STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l33 full
FULL SEARCH INITIATED 14:35:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1185 TO ITERATE

100.0% PROCESSED   1185 ITERATIONS   0 ANSWERS
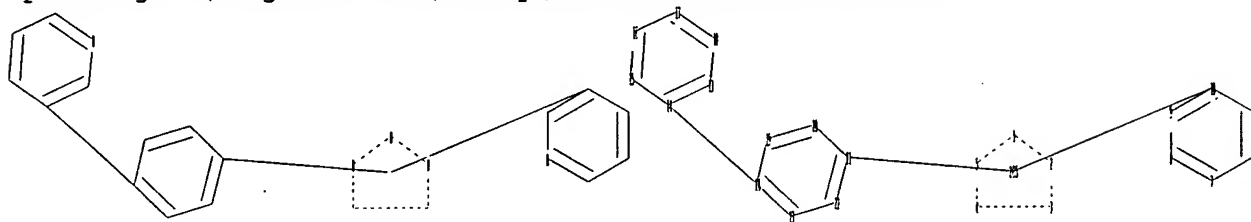SEARCH TIME: 00.00.01

L34   0 SEA SSS FUL L33

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res19.str

ring nodes :
1 2 3 4 5   7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
14-24
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
14-24
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

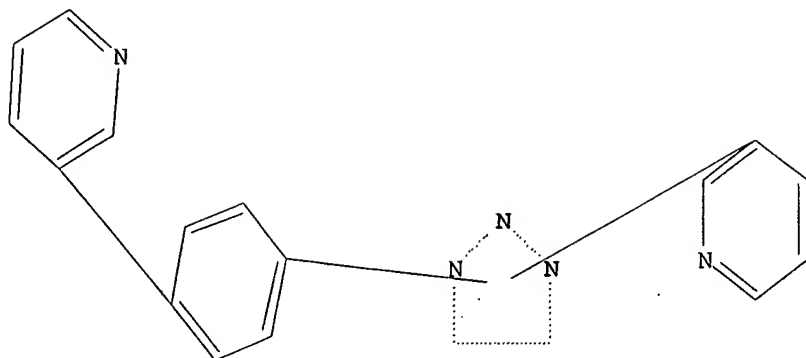L35   STRUCTURE UPLOADED

=> d
L35 HAS NO ANSWERS
L35   STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l35 full
FULL SEARCH INITIATED 14:35:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
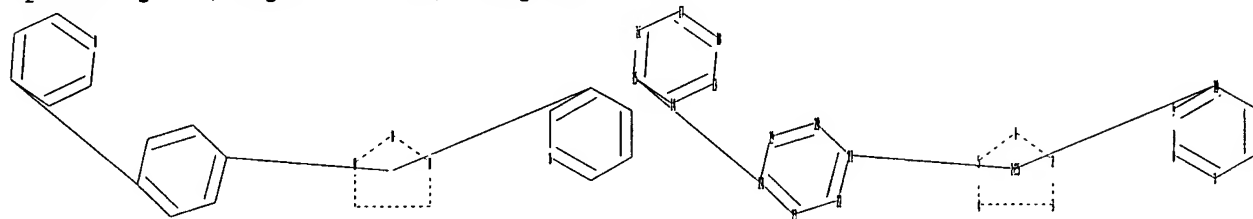SEARCH TIME: 00.00.01

L36   0 SEA SSS FUL L35

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res20.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
15-24
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
15-24
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

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Match level :
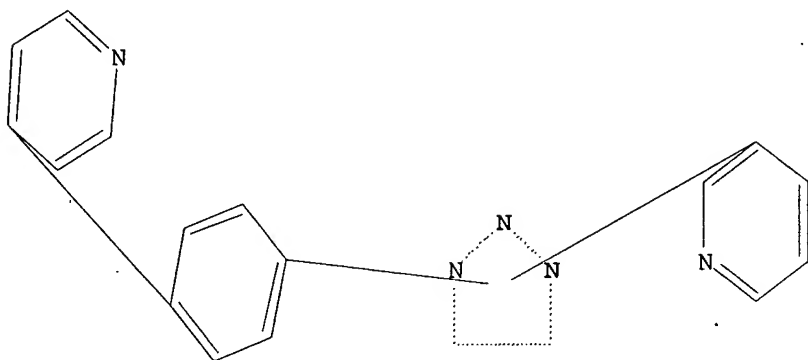1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom

L37   STRUCTURE UPLOADED

=> d
L37 HAS NO ANSWERS
L37   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l37 full
FULL SEARCH INITIATED 14:36:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   435 TO ITERATE

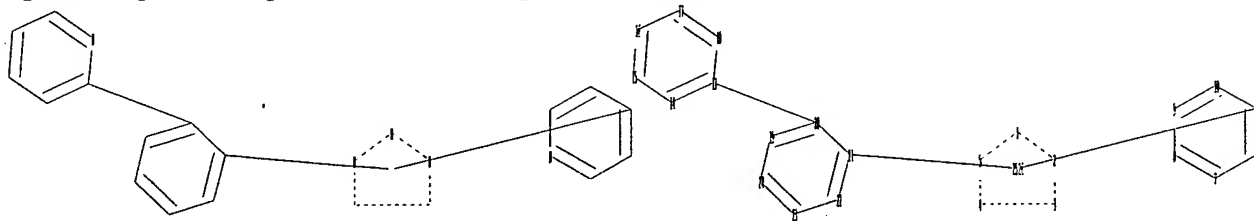100.0% PROCESSED   435 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L38   0 SEA SSS FUL L37

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res21.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :

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13-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
13-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
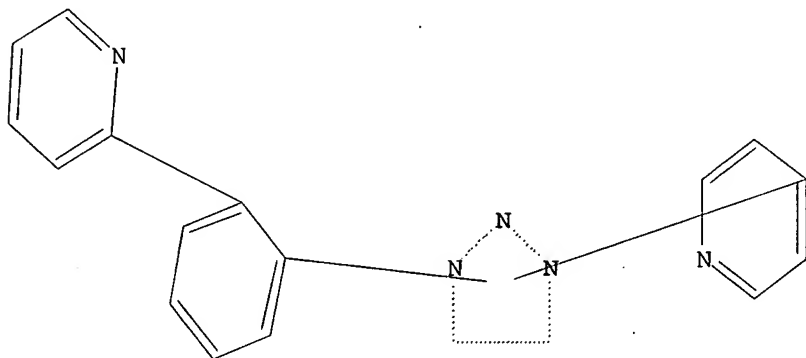containing 1 : 7 : 13 : 19 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L39   STRUCTURE UPLOADED

=> d
L39 HAS NO ANSWERS
L39   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l39 full
FULL SEARCH INITIATED 14:37:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1185 TO ITERATE

100.0% PROCESSED   1185 ITERATIONS   0 ANSWERS
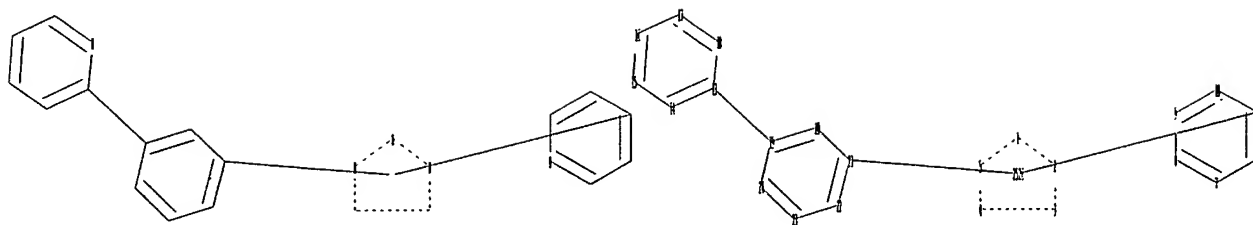SEARCH TIME: 00.00.01

L40   0 SEA SSS FUL L39

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res22.str

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```
ring nodes :
1   2   3   4   5   7   8   9   10  11  12  13  14  15  16  17  18  19  20  21  22  23  24
chain bonds :
13-19
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15
15-16   16-17   17-18   19-24   19-20   20-21   21-22   22-23   23-24
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
13-19
normalized bonds :
7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15   15-16   16-17   17-18   19-24
 19-20   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :


Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom
```
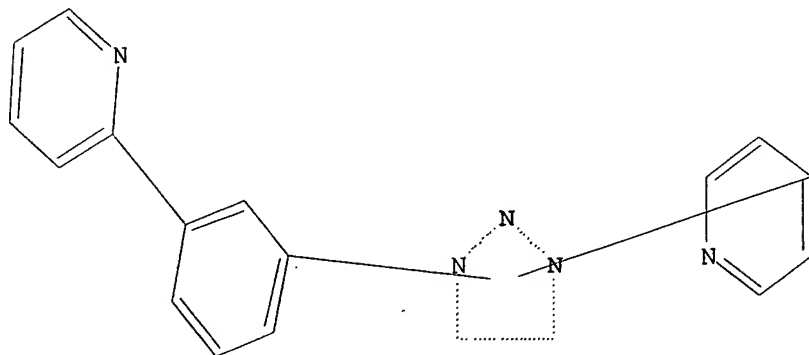
L41   STRUCTURE UPLOADED

```
=> d
L41 HAS NO ANSWERS
L41              STR
```


Karen Cheng

10552362a

Structure attributes must be viewed using STN Express query preparation.


```
=> s l41 full
FULL SEARCH INITIATED 14:38:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1185 TO ITERATE

100.0% PROCESSED     1185 ITERATIONS                    0 ANSWERS
SEARCH TIME: 00.00.01

L42           0 SEA SSS FUL L41

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res23.str
```
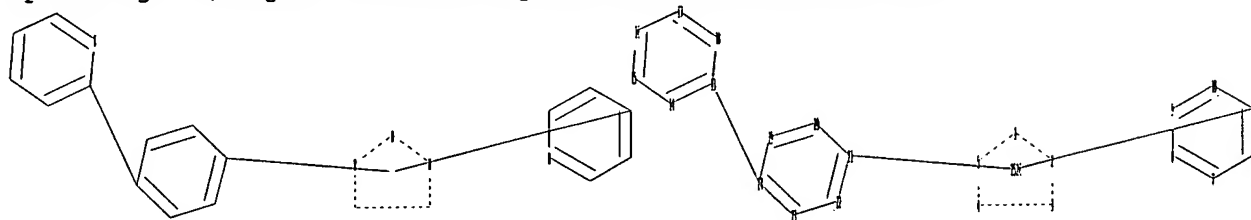


```
ring nodes :
1  2  3  4  5  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23  24
chain bonds :
13-24
ring bonds :
1-2  1-5  2-3  3-4  4-5  7-8  7-12  8-9  9-10  10-11  11-12  13-18  13-14  14-15
15-16  16-17  17-18  19-24  19-20  20-21  21-22  22-23  23-24
exact/norm bonds :
1-2  1-5  2-3  3-4  4-5
exact bonds :
13-24
normalized bonds :
7-8  7-12  8-9  9-10  10-11  11-12  13-18  13-14  14-15  15-16  16-17  17-18  19-24
 19-20  20-21  21-22  22-23  23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  7:Atom  8:Atom  9:Atom  10:Atom  11:Atom
12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom
21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom



L43      STRUCTURE UPLOADED

=> d
L43 HAS NO ANSWERS
L43               STR
```
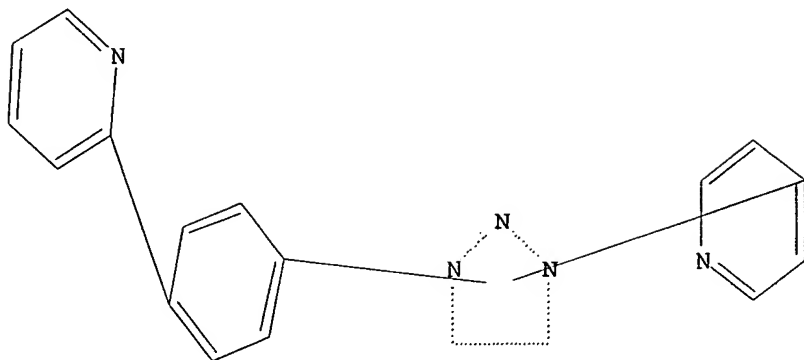

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Structure attributes must be viewed using STN Express query preparation.


```
=> s 143 full
FULL SEARCH INITIATED 14:38:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      1185 TO ITERATE

100.0% PROCESSED     1185 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01

L44             0 SEA SSS FUL L43

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res24.str
```
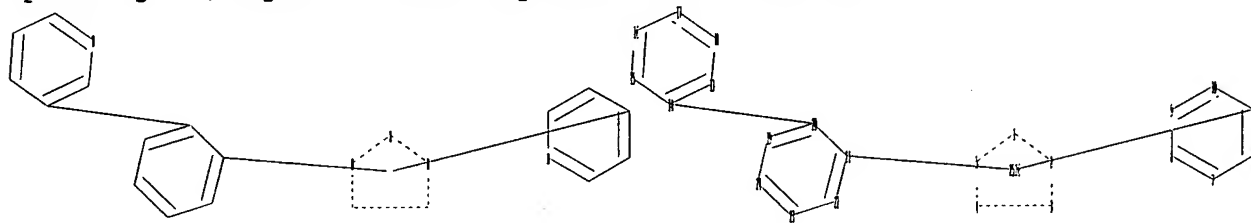


```
ring nodes :
1  2   3   4   5   7   8   9   10  11  12  13  14  15  16  17  18  19  20  21  22  23  24
chain bonds :
14-20
ring bonds :
1-2  1-5  2-3  3-4  4-5  7-8  7-12  8-9  9-10  10-11  11-12  13-18  13-14  14-15
15-16  16-17  17-18  19-24  19-20  20-21  21-22  22-23  23-24
exact/norm bonds :
1-2  1-5  2-3  3-4   4-5
exact bonds :
14-20
normalized bonds :
7-8  7-12  8-9  9-10  10-11  11-12  13-18  13-14  14-15  15-16  16-17  17-18  19-24
 19-20  20-21  21-22  22-23  23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :
```


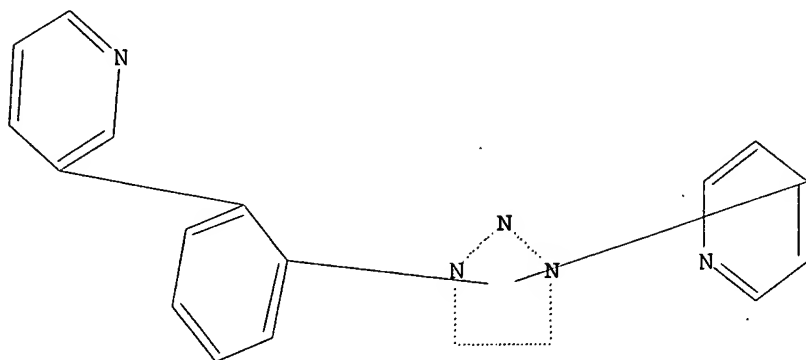Karen Cheng

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L45   STRUCTURE UPLOADED

=> d
L45 HAS NO ANSWERS
L45   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l45 full
FULL SEARCH INITIATED 14:39:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
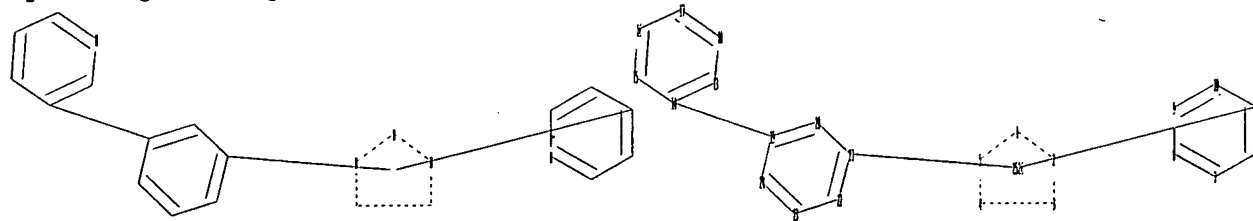SEARCH TIME: 00.00.01

L46   0 SEA SSS FUL L45

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res25.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :

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14-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
14-19
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
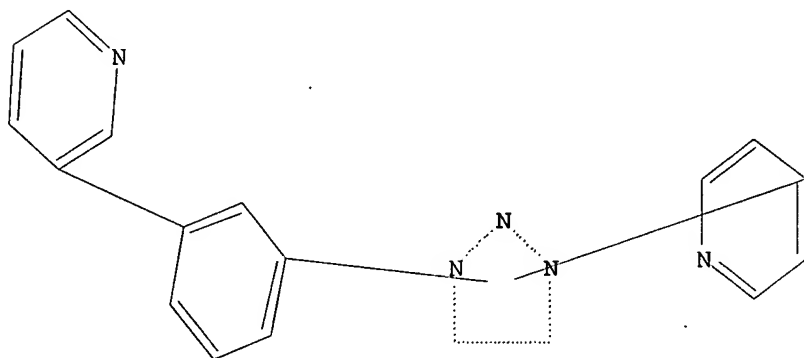containing 1 : 7 : 13 : 19 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L47   STRUCTURE UPLOADED

=> d
L47 HAS NO ANSWERS
L47   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l47 full
FULL SEARCH INITIATED 14:40:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
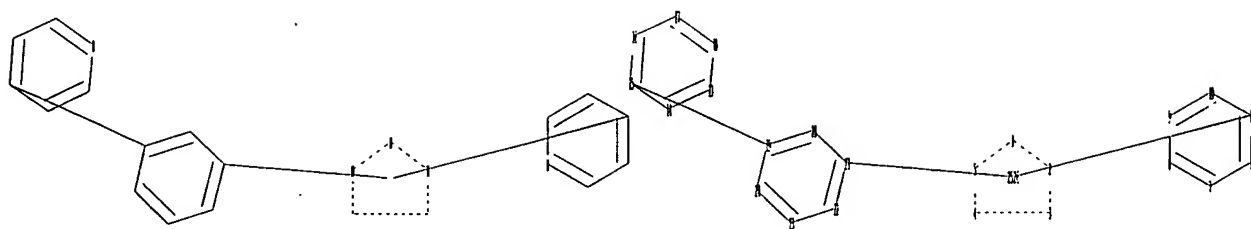SEARCH TIME: 00.00.01

L48   0 SEA SSS FUL L47

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res26.str

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ring nodes :
1   2   3   4   5   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22   23   24
chain bonds :
15-19
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15
15-16   16-17   17-18   19-24   19-20   20-21   21-22   22-23   23-24
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
15-19
normalized bonds :
7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15   15-16   16-17   17-18   19-24
 19-20   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

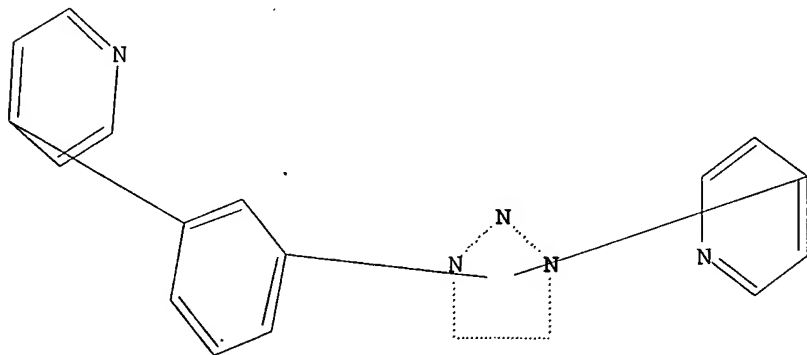Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom

L49   STRUCTURE UPLOADED

=> d
L49 HAS NO ANSWERS
L49   STR

Karen Cheng

10552362a

Structure attributes must be viewed using STN Express query preparation.


```
=> s l49 full
FULL SEARCH INITIATED 14:40:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     435 TO ITERATE

100.0% PROCESSED      435 ITERATIONS                    0 ANSWERS
SEARCH TIME: 00.00.01

L50              0 SEA SSS FUL L49

=>
```
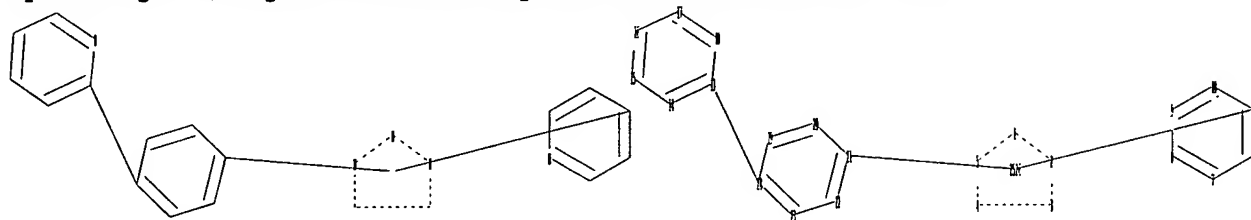Uploading C:\Program Files\Stnexp\Queries\10552362res27.str


```
ring nodes :
1  2  3  4  5  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23  24
chain bonds :
13-24
ring bonds :
1-2  1-5  2-3  3-4  4-5  7-8  7-12  8-9  9-10  10-11  11-12  13-18  13-14  14-15
15-16  16-17  17-18  19-24  19-20  20-21  21-22  22-23  23-24
exact/norm bonds :
1-2  1-5  2-3  3-4  4-5
exact bonds :
13-24
normalized bonds :
7-8  7-12  8-9  9-10  10-11  11-12  13-18  13-14  14-15  15-16  16-17  17-18  19-24
 19-20  20-21  21-22  22-23  23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  7:Atom  8:Atom  9:Atom  10:Atom  11:Atom
12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom
21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom


L51      STRUCTURE UPLOADED

=> s l51 full
FULL SEARCH INITIATED 14:41:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1185 TO ITERATE
```


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100.0% PROCESSED   1185 ITERATIONS   0 ANSWERS
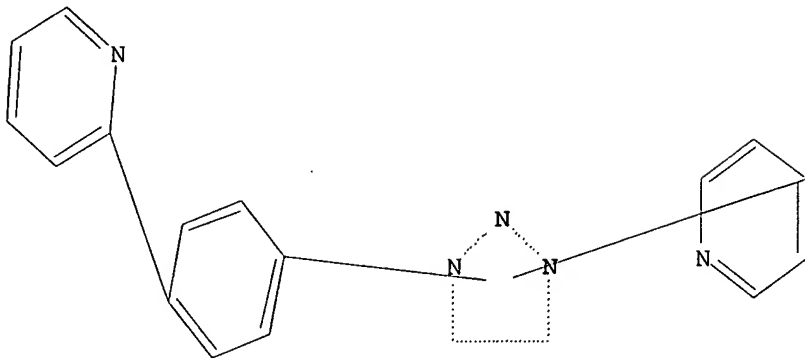SEARCH TIME: 00.00.01

L52   0 SEA SSS FUL L51

=> d l51
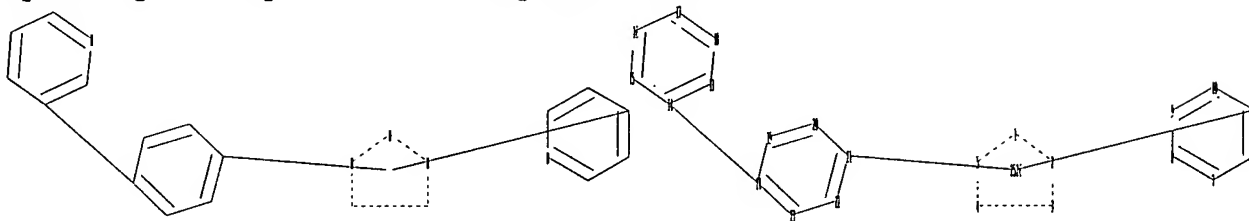L51 HAS NO ANSWERS
L51   STR

Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res28.str

ring nodes :
1 2 3 4 5   7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
14-24
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
14-24
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

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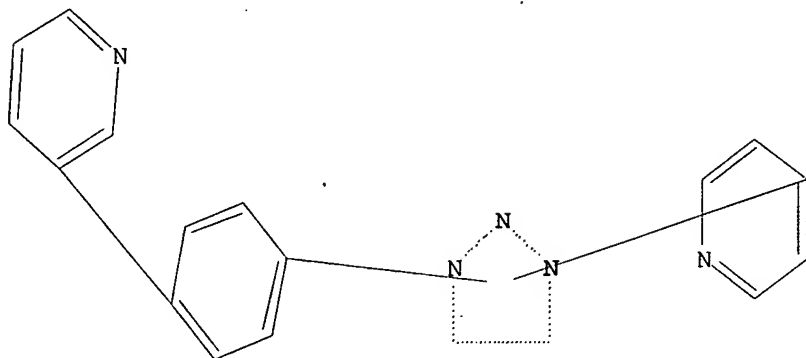10552362a

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom   20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L53   STRUCTURE UPLOADED

=> d
L53 HAS NO ANSWERS
L53   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l53 full
FULL SEARCH INITIATED 14:42:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   614 TO ITERATE

100.0% PROCESSED   614 ITERATIONS   0 ANSWERS
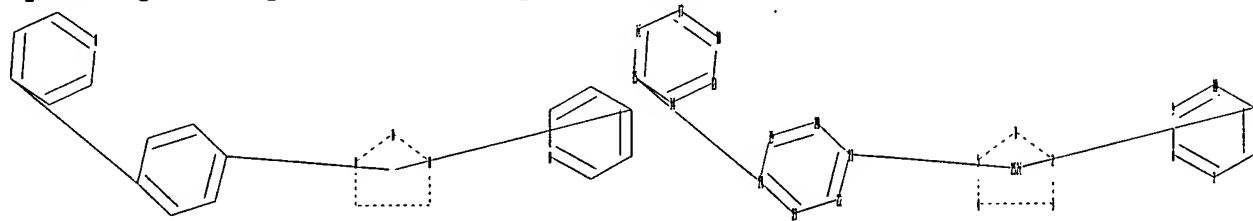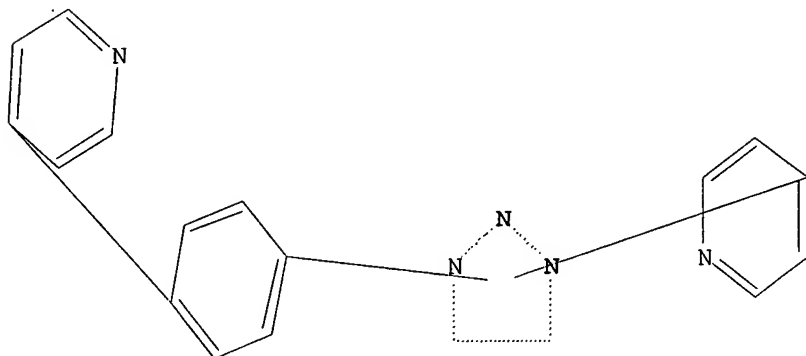SEARCH TIME: 00.00.01

L54   0 SEA SSS FUL L53

=>
Uploading C:\Program Files\Stnexp\Queries\10552362res29.str

ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :

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15-24
ring bonds :
1-2   1-5   2-3   3-4   4-5   7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15
15-16   16-17   17-18   19-24   19-20   20-21   21-22   22-23   23-24
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5
exact bonds :
15-24
normalized bonds :
7-8   7-12   8-9   9-10   10-11   11-12   13-18   13-14   14-15   15-16   16-17   17-18   19-24
 19-20   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom
21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom

L55   STRUCTURE UPLOADED

=> d
L55 HAS NO ANSWERS
L55   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l55 full
FULL SEARCH INITIATED 14:42:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   435 TO ITERATE

100.0% PROCESSED   435 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L56   0 SEA SSS FUL L55

=> fil caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                            ENTRY   SESSION

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=> d his

        (FILE 'HOME' ENTERED AT 14:20:17 ON 02 APR 2007)

        FILE 'REGISTRY' ENTERED AT 14:20:27 ON 02 APR 2007
L1   STRUCTURE UPLOADED
L2   0 S L1 FULL
L3   STRUCTURE UPLOADED
L4   2 S L3 FULL
L5   STRUCTURE UPLOADED
L6   STRUCTURE UPLOADED
L7   8 S L6 FULL
L8   STRUCTURE UPLOADED
L9   0 S L8 FULL
L10   STRUCTURE UPLOADED
L11   2 S L10 FULL
L12   STRUCTURE UPLOADED
L13   0 S L12 FULL
L14   STRUCTURE UPLOADED
L15   0 S L14 FULL
L16   STRUCTURE UPLOADED
L17   STRUCTURE UPLOADED
L18   0 S L17 FULL
L19   STRUCTURE UPLOADED
L20   0 S L19 FULL
L21   STRUCTURE UPLOADED
L22   0 S L21 FULL
L23   STRUCTURE UPLOADED
L24   0 S L23 FULL
L25   STRUCTURE UPLOADED
L26   0 S L25 FULL
L27   STRUCTURE UPLOADED
L28   0 S L27 FULL
L29   STRUCTURE UPLOADED

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```
L30            0 S L29 FULL
L31              STRUCTURE UPLOADED
L32            0 S L31 FULL
L33              STRUCTURE UPLOADED
L34            0 S L33 FULL
L35              STRUCTURE UPLOADED
L36            0 S L35 FULL
L37              STRUCTURE UPLOADED
L38            0 S L37 FULL
L39              STRUCTURE UPLOADED
L40            0 S L39 FULL
L41              STRUCTURE UPLOADED
L42            0 S L41 FULL
L43              STRUCTURE UPLOADED
L44            0 S L43 FULL
L45              STRUCTURE UPLOADED
L46            0 S L45 FULL
L47              STRUCTURE UPLOADED
L48            0 S L47 FULL
L49              STRUCTURE UPLOADED
L50            0 S L49 FULL
L51              STRUCTURE UPLOADED
L52            0 S L51 FULL
L53              STRUCTURE UPLOADED
L54            0 S L53 FULL
L55              STRUCTURE UPLOADED
L56            0 S L55 FULL

       FILE 'CAPLUS' ENTERED AT 14:42:52 ON 02 APR 2007

=> s (l4 or l7 or l11)
               1 L4
               1 L7
               1 L11
L57            1 (L4 OR L7 OR L11)

=> d ibib abs hitstr tot
```
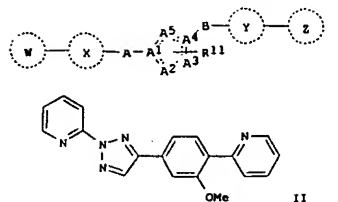
Karen Cheng

10552362a

ACCESSION NUMBER: 2004:878275 CAPLUS
DOCUMENT NUMBER: 141:366235
TITLE: Preparation of diaryl substituted triazole modulators
                       of metabotropic glutamate receptor-5
INVENTOR(S):   Cosford, Nicholas D. P.; Roppe, Jeffrey R.; Tehrani,
                       Lida R.; Wang, Bowei
PATENT ASSIGNEE(S):   Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 42 pp.
                       CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089306	A2	20041021	WO 2004-US9750	20040331
WO 2004089306	A3	20050217		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
    CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
    GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
    LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
    NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
    TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
    BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
    ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
    SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
    TD, TG

AU 2004227833	A1	20041021	AU 2004-227833	20040331
CA 2521396	A1	20041021	CA 2004-2521396	20040331
EP 1613617	A2	20060111	EP 2004-758603	20040331

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
    IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK

| CN 1795186 | A | 20060628 | CN 2004-80014560 | 20040331 |
| JP 2006522131 | T | 20060928 | JP 2006-509488 | 20040331 |

PRIORITY APPLN. INFO.:   US 2003-462796P   P 20030404

                                               WO 2004-US9750   W 20040331
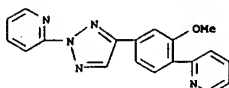
OTHER SOURCE(S):   MARPAT 141:366235
GI

II

AB   Title compds. represented by the formula I [wherein X, Y = independently
     (hetero)aryl, and at least one of X and Y is a heteroaryl with N adjacent
     to the position of attachment to A or B; A1-A5 = independently N or C,
     three of them are N, and one of A1 and A4 must be N, but not both A1 and
     A4 are N; A, B = independently (hetero)alkyl, alkylsulfonylalkyl,
     alkylcarbonylalkyl, etc.; W, Z = independently (un)substituted
     (hetero)cycloalkyl, alkyl(hetero)aryl; R11 = halo, alkyl, alkoxyl, etc.;
     and pharmaceutically acceptable salts thereof] were prepared as
     modulators
     of metabotropic glutamate receptor-5 (mGluR5). For example, reaction of
     2-[2-methoxy-4-(1H-1,2,3-triazol-4-yl)phenyl]pyridine with
     1-fluoropyridinium triflate gave II. The prepared I were tested for
     mGluR5
     inhibitory activity with IC50 value of less than 10 μM in the calcium
     flux assay or inhibition of >50 % at a concentration of 100 μM in the PI
     assay. Thus, I and their pharmaceutical compns. are useful as modulators
     of mGluR5 for the treatment of panic, and bipolar disorder, as well as in
     the treatment of psychiatric and mood disorders such as, for example,
     schizophrenia, anxiety, depression, panic, and bipolar disorder, as well
     as in the treatment of pain, Parkinson's disease, cognitive dysfunction,
     epilepsy, circadian rhythm disorders, obesity, drug addiction, drug
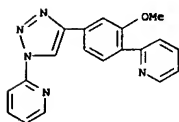   abuse,
     drug withdrawal and other diseases (no data).
IT   777864-97-8P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of diaryl substituted triazole modulators of metabotropic
        glutamate receptor-5)
RN   777864-97-8 CAPLUS
CN   Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]-,
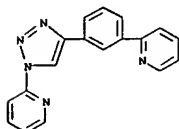   monohydrochloride (9CI) (CA INDEX NAME)

● HCl

IT   777864-98-9P 777864-99-0P 777865-00-6P
     777865-01-7P 777865-02-8P 777865-03-9P
     777865-04-0P 777865-05-1P 777865-06-2P
     777865-08-4P 777865-09-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of diaryl substituted triazole modulators of metabotropic
        glutamate receptor-5)
RN   777864-98-9 CAPLUS
CN   Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]-,
     monohydrochloride (9CI) (CA INDEX NAME)
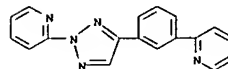

● HCl

RN   777864-99-0 CAPLUS
CN   Pyridine, 2-[4-[3-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]- (9CI) (CA
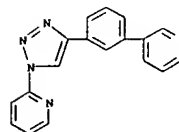   INDEX NAME)
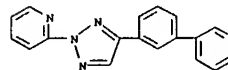

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RN   777865-00-6 CAPLUS
CN   Pyridine, 2-[4-[3-(2-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]- (9CI) (CA
     INDEX NAME)

RN   777865-01-7 CAPLUS
CN   Pyridine, 2-[4-[3-(3-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]- (9CI) (CA
     INDEX NAME)

RN   777865-02-8 CAPLUS
CN   Pyridine, 2-[4-[3-(3-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]- (9CI) (CA
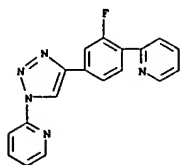   INDEX NAME)

RN   777865-03-9 CAPLUS
CN   Pyridine, 2-[4-[3-fluoro-4-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]-
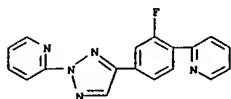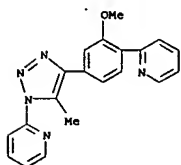   (9CI) (CA INDEX NAME)

10552362a

RN   777865-04-0 CAPLUS
CN   Pyridine, 2-[4-[3-fluoro-4-(2-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]-
      (9CI) (CA INDEX NAME)
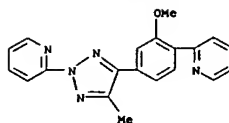
RN   777865-05-1 CAPLUS
CN   Pyridine, 2-[2-methoxy-4-[5-methyl-1-(2-pyridinyl)-1H-1,2,3-triazol-4-
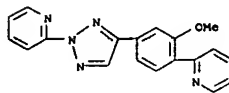   yl]phenyl]- (9CI) (CA INDEX NAME)

RN   777865-06-2 CAPLUS
CN   Pyridine, 2-[2-methoxy-4-[5-methyl-2-(2-pyridinyl)-2H-1,2,3-triazol-4-
      yl]phenyl]- (9CI) (CA INDEX NAME)

RN   777865-08-4 CAPLUS
CN   Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]-
      (9CI) (CA INDEX NAME)

RN   777865-09-5 CAPLUS
CN   Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]-
      (9CI) (CA INDEX NAME)

Karen Cheng